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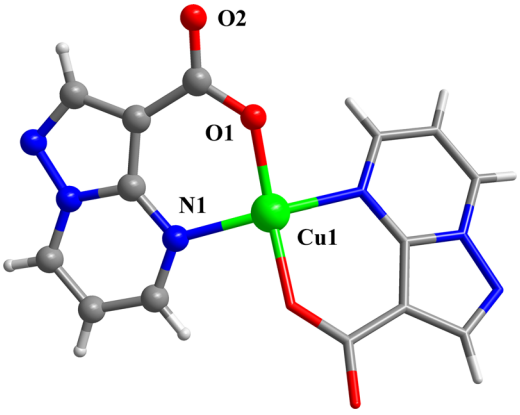
The crystal structure of bis(pyrazolo[1,5-*a*]pyrimidine-3-carboxylato-κ^2N,O)-copper(II), $C_{14}H_8N_6O_4Cu$



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Abstract

$C_{14}H_8N_6O_4Cu$, monoclinic, *C*2/*c* (no. 15), a = 15.6054(8) Å, b = 7.0441(3) Å, c = 12.6301(6) Å, β = 108.550(5)°, V = 1316.24(11) Å^3, Z = 4, $R_{gt}(F)$ = 0.0317, $wR_{ref}(F^2)$ = 0.0778, T = 293 K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

All reagents were commercially available and used as purchased without further purification. The title complex was prepared under the mild hydrothermal condition by the following procedure: a mixture of pyrazolo[1,5-*a*]pyrimidine-3-carboxylic acid (32.6 mg, 0.2 mmol), $Cu(CH_3COO)_2{\cdot}H_2O$ (39.9 mg, 0.2 mmol) and 5 mL deionized water was sealed in a 25 mL Teflon-lined stainless steel vessel and heated at 353 K for 3 days under autogenous pressure. Then the reaction was then stopped and cooled down to room temperature and filtered. Blue block crystals of title complex were obtained (yield: 51% based on Cu).

Table 1: Data collection and handling.

Crystal:	Blue block
Size:	0.35 × 0.34 × 0.30 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	1.70 mm^{-1}
Diffractometer, scan mode:	SuperNova, ω
θ_{max}, completeness:	29.4°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	7521, 1631, 0.035
Criterion for I_{obs}, $N(hkl)_{gt}$:	I_{obs} > 2 σ(I_{obs}), 1460
$N(param)_{refined}$:	114
Programs:	CrysAlis^{PRO} [1], SHELX [2, 3], Olex2 [4]

Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

Comment

The synthesis and characterization of copper complexes have attracted tremendous attention over the past decades owing to their potential applications [5–8]. In this context, a variety of copper(II) complexes ranging from discrete and extended structures have been synthesized. The text book knowledge organic carboxylate ligands containing additional N- or O-coordinating sites are vastly used because they can chelate as well as bridge copper(II) ions to construct discrete and extended structures [9–13]. Considering its structure, the rigid pyrazolo[1,5-*a*]pyrimidine-3- carboxylate anion can provide both nitrogen atoms and the oxygen atoms for coordination with metal atoms, which makes it a useful ligand. Herein, we describe the

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.5000	0.21781(5)	0.7500	0.01938 (13)
O1	0.40439 (10)	0.1527 (2)	0.61711 (12)	0.0247 (3)
O2	0.33477 (10)	0.0902 (2)	0.43799 (13)	0.0280 (4)
N1	0.59021 (12)	0.2811 (3)	0.67478 (14)	0.0189 (4)
N2	0.61305 (12)	0.3513 (3)	0.50131 (14)	0.0199 (4)
N3	0.56928 (13)	0.3449 (3)	0.38898 (15)	0.0262 (4)
C1	0.39972 (14)	0.1533 (3)	0.51255 (17)	0.0187 (4)
C2	0.47766 (14)	0.2343 (3)	0.48592 (17)	0.0181 (4)
C3	0.48836 (16)	0.2733 (3)	0.38201 (18)	0.0234 (5)
H3	0.4433	0.2514	0.3144	0.028*
C4	0.55932 (14)	0.2860 (3)	0.56175 (17)	0.0172 (4)
C5	0.69864 (14)	0.4136 (3)	0.55167 (19)	0.0243 (5)
H5	0.7340	0.4599	0.5105	0.029*
C6	0.73036 (15)	0.4054 (3)	0.6652 (2)	0.0276 (5)
H6	0.7891	0.4438	0.7032	0.033*
C7	0.67439 (15)	0.3389 (3)	0.72479 (18)	0.0239 (5)
H7	0.6971	0.3351	0.8023	0.029*

synthesis and structural characterization of a mononuclear copper complex based on the pyrazolo[1,5-*a*]pyrimidine-3-carboxylic acid.

The title complex, $C_{14}H_8N_6O_4Cu$, was synthesized using pyrazolo[1,5-*a*]pyrimidine-3-carboxylic acid and $Cu(CH_3COO)_2{\cdot}H_2O$ under mild hydrothermal condition. X-ray structural analysis shows that the complex crystallizes in the monoclinic space group *C*2/*c*. The asymmetric unit of the title crystal structure contains half a Cu^{2+} ion (located on a twofold axis; see the figure) and one fully deprotonated pyrazolo[1,5-*a*]pyrimidine-3-carboxylate anion. The Cu(II) ion is four-coordinated with two carboxylate O atoms (Cu1–O1 = 1.9131(14) Å) and two pyridine N atoms (Cu1–N1 = 1.9835(18) Å) from two pyrazolo[1,5-*a*] pyrimidine-3-carboxylate ligands, forming a square-planar geometry. The Cu–O/N distances are within the normal ranges.

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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